

# Geometrical Properties of Cumulant Expansions

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## Abstract

Cumulants represent a natural language for expressing macroscopic properties of a solid. We show that cumulants are subject to a nontrivial geometry. This geometry provides an intuitive understanding of a number of cumulant relations which had been obtained so far by using algebraic considerations. We give general expressions for their infinitesimal and finite transformations and represent a cumulant wave operator through an integration over a path in the Hilbert space. Cases are investigated where this integration can be done exactly. An expression of the ground-state wavefunction in terms of the cumulant wave operator is derived. In the second part of the article we derive the cumulant counterpart of Faddeev's equations and show its connection to the method of increments.

## I. INTRODUCTION

In statistical physics, quantum mechanics, quantum field theory and many other fields of modern theoretical physics we constantly face objects of the type

$$F = \ln \langle e^{\lambda_1 A_1 + \lambda_2 A_2 + \dots} \rangle. \quad (1)$$

Here  $A_1, A_2, \dots$  are abstract elements,  $\lambda_1, \lambda_2, \dots$  are numbers,  $\langle \dots \rangle$  means some kind of averaging and  $e^{(\dots)}$  denotes a generalized exponential function.

Assuming the average of 1 to be nonzero, we conclude that  $F$  is an analytic function of the  $\lambda_i$  in a vicinity of zero. Therefore, it has a Taylor expansion with respect to the  $\lambda_i$ . This expansion is called *cumulant expansion*, the coefficients of the expansion are called *cumulants*.

*Cumulants (semiinvariants)* have been known long before in mathematical statistics and probability theory. Kubo [1] pioneered in demonstrating their usefulness in diverse branches of physics. Considered as abstract objects cumulants form a special kind of noncommuting algebra. In his original paper Kubo applied relations found in this algebra to a diverse set of physical problems. In particular, he gave an elegant derivation of the Ursell-Mayer expansion for classical and quantum gases that is usually obtained by much longer diagram considerations, he rederived Goldstone perturbation theory for the ground-state of a Hamilton operator, and investigated the motion of an oscillator with a random frequency. Kubo stressed the idea that "the generalized cumulant expansion provides us with a point of view from which many existent methods in quantum mechanics and statistical physics can be unified" [1].

Cumulants found a fundamental application in solid-state physics [2] (and references therein), [3], [4], [5], [6] as a universal language for expressing properties of a solid in a *size-consistent* way. Expressions for the ground-state energy, expectation values of operators, correlation functions and other quantities characterizing a solid were derived by applying the cumulant technique. These expressions remain valid in the strongly correlated case, when the ground-state of the unperturbed Hamiltonian is not a single particle one and the usual diagrammatic theory based on Wick theorem either breaks down or becomes very complicated. Also, an important feature is that any cumulant expression vanishes for statistically independent processes. Thus the cumulant technique takes into account only relevant, statistically connected terms, e.g., of perturbation theory.

In this article we continue exploring the cumulant technique and show that cumulants possess a nontrivial geometry. This geometry helps to make clear and intuitive results obtained before by using algebraic considerations. Geometry in an abstract sense means

studying how the properties of objects change under transformations [7]. First, we find a formula for an infinitesimal transformation of a cumulant, and then integrate it in order to obtain a finite transformation.

It comes out that a transformation of a cumulant expression corresponds to a multiplication by some *cumulant wave operator*  $\Omega$ . Different analytical expressions for  $\Omega$  were obtained before through cumulant algebra [2]. We give a general expression for  $\Omega$  through an integration over a path in Hilbert space, and show cases when this integration can be done analytically. Then we investigate the ground-state wavefunction of a Hamilton operator and give an expression for it by applying cumulant technique. For this we first need to add a new element to the cumulant algebra which is the cumulant of the number 1. Next we show how the cumulant expressions found before can be rederived by using geometrical considerations. This includes orthogonality relations for  $\Omega$ , for the ground-state energy, and for expectation values of operators and correlation functions. Then we give some new applications of the cumulant technique.

First we show how improved short-time propagators for quantum Monte Carlo methods can be derived by using cumulant expansions and derive high-order approximations for coordinate-momentum and coordinate-coordinate propagators. Then we consider the foundation of the method of increments and extend this method to excited states of a Hamilton operator. The method of increments has been proven a powerful and intuitive way of taking into account electron correlations in solids [8], [9], [10], [11], [12], [13]. The existing theoretical justification of the method of increments is based on Bethe-Goldstone equations. The  $n$ -th order Bethe-Goldstone equation is equivalent to a variational calculation with some trial wavefunction (for the explicit construction of this function see [14]). This makes the Bethe-Goldstone equations approximate by nature. Therefore, although the Bethe-Goldstone equations provide a justification for the method of increments, they are not able to predict what part of the problem is neglected by performing an  $n$ -th order increment calculation. In other words, we do not have an exact  $n$ -th order equation, such that the  $n$ -th order increment equation would be an approximation to this equation. Also we should make

a remark that the  $n$ -th order Bethe-Goldstone equation is restricted to a vacuum taken as the unperturbed state. Therefore, it is not applicable when we need to take into account additional correlations starting from an already correlated state.

On the other hand *Faddeev's equations for the 3-body problem* are well known [15], [16] and have been successfully applied in nuclear physics [17] and in solid-state theory [18], [19], [20], [21]. Faddeev's equations are *exact*, this feature makes their application mathematically controllable. We show that we are able to generate a hierarchy of Faddeev-like cumulant equations. Taking the equation of the  $n$ -th order in the leading approximation we exactly recover the  $n$ -th order increment expansion. We can see explicitly from the  $n$ -th order cumulant Faddeev's equation what part is neglected by the increment approximation. Therefore, we generally predict the validity and the precision of the  $n$ -th order increment calculation. The cumulant Faddeev's equations enable us to formulate an increment method for excited states of a Hamilton operator.

Finally, we give the conclusions and point out future directions of research.

## II. GEOMETRICAL PROPERTIES OF CUMULANTS

### A. Definitions and properties

We start by defining the cumulant of  $N$  operators [2].

**Definition 1** *The cumulant of  $N$  operators is defined as*

$$\langle A_1 \dots A_N \rangle^c = \frac{\partial}{\partial \lambda_1} \dots \frac{\partial}{\partial \lambda_N} \bigg|_{\lambda_1 = \dots = \lambda_N = 0} \ln \langle x | e^{\lambda_1 A_1} \dots e^{\lambda_N A_N} | y \rangle. \quad (2)$$

Here  $x, y$  are vectors belonging to the Hilbert space, we suppose  $\langle x | y \rangle \neq 0$ .

We denote this cumulant as  $\langle A_1 \dots A_N \rangle^c$  or, when we need to give the averaging vectors  $x$  and  $y$  explicitly, as  $\langle x | A_1 \dots A_N | y \rangle^c$ .

Cumulants possess a number of properties (see [2]). We briefly repeat them below. To simplify notations we consider the case of a two-operator cumulant.

1. Linearity:

$$\langle A(\alpha B + \beta C) \rangle^c = \alpha \langle AB \rangle^c + \beta \langle AC \rangle^c.$$

2. Independence of the norm of the averaging vectors:

$$\langle \epsilon x \mid AB \mid y \rangle^c = \langle x \mid AB \mid y \rangle^c \quad \text{for } \epsilon \neq 0.$$

3. Operators  $A$  and  $B$  are called *statistically independent* with respect to  $x, y$  when the average of their product is equal to the product of their averages, i.e.,

$$\langle x \mid AB \mid y \rangle = \langle x \mid A \mid y \rangle \langle x \mid B \mid y \rangle, \quad \langle x \mid y \rangle = 1.$$

Then

$$\langle x \mid AB \mid y \rangle^c \equiv 0.$$

4. Applying Definition 1 we can obtain explicit formulas for cumulants. For the case  $\langle x \mid y \rangle = 1$  they read as

$$\langle x \mid A \mid y \rangle^c = \langle x \mid A \mid y \rangle$$

$$\langle x \mid AB \mid y \rangle^c = \langle x \mid AB \mid y \rangle - \langle x \mid A \mid y \rangle \langle x \mid B \mid y \rangle, \text{ etc.}$$

5. We need to distinguish the cumulant of two operators  $A$  and  $B$  and the cumulant of an operator  $AB$  considered as an entity, when cumulants are evaluated. The latter one we denote as  $\langle (AB)^\bullet \rangle$ .

Also we need to distinguish between the number 1 and the unit operator  $\mathbf{1}$ . For instance  $\langle 1 \cdot A \rangle^c = \langle A \rangle^c$  and  $\langle \mathbf{1}A \rangle^c \equiv 0$ .

We define *formal powers* as  $\langle A^n \rangle^c = \langle \underbrace{A \dots A}_n \rangle^c$ . Then the *formal algebra* of power series must be considered.

Let us formulate an important statement.

**Statement 1** *Let  $H$  be a Hamilton operator. Let  $\psi$  be an eigenvector of this operator with an eigenvalue  $E$ . Then for any vector  $\psi_0$ ,  $\langle \psi_0 | \psi \rangle \neq 0$  and for any cumulant series  $A$ , not including  $c$ -numbers the following relations hold*

$$\langle \psi_0 | H | \psi \rangle^c = E \quad (3)$$

$$\langle \psi_0 | AH | \psi \rangle^c = 0. \quad (4)$$

*Proof:*

The proof of (3) comes from the definition of a cumulant of one operator. Equation (4) follows from the fact, that  $H$  acting on  $|\psi\rangle$  leads to a multiplication by a number and therefore the logarithm in (2) factorizes.

The opposite statement is also true:

**Statement 2** *Let*

$$\langle \psi_0 | AH | \psi \rangle^c = 0$$

*for any  $\psi_0$ ,  $\langle \psi_0 | \psi \rangle \neq 0$  and for any  $A$  not including  $c$ -numbers.*

*Then  $\psi$  is an eigenvector of  $H$ .*

*Proof:*

Let  $P$  be a projecting operator on the direction of  $\psi$ . Without loss of generality we assume  $\langle \psi_0 | \psi \rangle = 1$ . Let us consider the following cumulant:

$$\langle \psi_0 | PH | \psi \rangle^c = \langle \psi_0 | PH | \psi \rangle - \langle \psi_0 | P | \psi \rangle \langle \psi_0 | H | \psi \rangle = \langle \psi_0 | PH - H | \psi \rangle.$$

Suppose  $\psi$  is not an eigenstate of  $H$ . Then  $(PH - H) | \psi \rangle \neq 0$ . Therefore we can choose a vector  $\psi_0$  such that  $\langle \psi_0 | PH | \psi \rangle^c \neq 0$ . But this contradicts the condition of the theorem. Therefore,  $\psi$  is an eigenstate of  $H$ .

## B. Transformations of averaging vectors

Here we analyse the basic geometric properties of cumulants. We show that a transformation of averaging vectors corresponds to a multiplication by the cumulant wave operator  $\Omega$  (for a definition of  $\Omega$  in terms of power series see [2]).

First we consider an *infinitesimal* transformation of one of the averaging vectors.

**Statement 3** *Let*

$$\psi_B = e^{\delta S} \psi_{B'} = (1 + \delta S) \psi_{B'}, \quad \delta S = \epsilon S, \quad \epsilon \ll 1.$$

*Then*

$$\langle \psi_A | X | \psi_B \rangle^c = \langle \psi_A | X(1 + \delta S) | \psi_{B'} \rangle^c. \quad (5)$$

*Here  $X$  is any formal cumulant series.*

*Proof:*

The proof follows from the definition of a cumulant. We present it for the case that  $X$  is a one-operator cumulant.

$$\begin{aligned} \langle \psi_A | X | \psi_B \rangle^c &= \frac{\partial}{\partial \lambda_{\lambda=0}} \ln \langle \psi_A | e^{\lambda X} | e^{\epsilon S} \psi_{B'} \rangle = \\ &= \frac{\partial}{\partial \lambda_{\lambda=0}} \ln \langle \psi_A | e^{\lambda X} | \psi_{B'} \rangle + \epsilon \frac{\partial}{\partial \epsilon_{\epsilon=0}} \frac{\partial}{\partial \lambda_{\lambda=0}} \ln \langle \psi_A | e^{\lambda X} e^{\epsilon S} | \psi_{B'} \rangle = \\ &= \langle \psi_A | X(1 + \delta S) | \psi_{B'} \rangle^c. \end{aligned}$$

Here we considered an infinitesimal transformation of the left averaging vector. In an analogous way, if for the right averaging vector

$$\psi_A = e^{\delta S} \psi_{A'} = (1 + \delta S) \psi_{A'}, \quad \delta S = \epsilon S, \quad \epsilon \ll 1$$

$$\text{then } \langle \psi_A | X | \psi_B \rangle^c = \langle \psi_{A'} | (1 + \delta S^\dagger) X | \psi_B \rangle^c.$$

We conclude that an infinitesimal transformation of the averaging vector result in a multiplication of the cumulant operator by  $1 + \delta S$ . In the following we call this operator *infinitesimal cumulant wave operator*.

The next step is going over to a finite transformation by integrating an infinitesimal one.

We consider the following construction:

**Construction 1** Let  $\psi_A, \psi_B, \psi_C$  be vectors of Hilbert space. Furthermore, let us consider a continuous path in Hilbert space between vectors  $\psi_B$  and  $\psi_C$ . Let us choose  $N + 1$  points  $\psi_0, \psi_1, \dots, \psi_N$  on this path such that  $\psi_0 = \psi_C$  and  $\psi_N = \psi_B$  and  $N$  operators  $\delta S_i$  such that  $\psi_i = e^{\delta S_i} \psi_{i-1}$ .

By assuming that the operators  $\delta S_i$  are small and using (5) we obtain

$$\langle \psi_A | X | \psi_B \rangle^c \approx \langle \psi_A | X \prod_{i=1}^N (1 + \delta S_i) | \psi_C \rangle^c.$$

Taking formally the limit  $N \rightarrow \infty$  we obtain

$$\langle \psi_A | X | \psi_B \rangle^c = \langle \psi_A | X \Omega | \psi_C \rangle^c$$

$$\Omega = \lim_{N \rightarrow \infty} \prod_{i=1}^N (1 + \delta S_i). \quad (6)$$

Thus we conclude that a transformation of an averaging vector in a cumulant expression corresponds to a multiplication with the operator  $\Omega$ . In the following we call this operator *cumulant wave operator*.

We note that there is a considerable freedom in the Construction 1 for choosing the path between vectors  $\psi_B, \psi_C$  and therefore the operators  $\delta S_i$ . Thus the operator  $\Omega$  is not defined uniquely. Two different representations for  $\Omega$  differ by a cumulant operator with a zero contribution to any cumulant expression (such operators can be obtained by integrating over a closed path in Hilbert space and subtracting the number 1).

We also note that  $\Omega$  always contains the number 1 as the first term of the formal series.

The formula for the finite transformation of the left averaging vector is obtained in analogy to (6). In that case we have



$$\langle \psi_A | X | \psi_B \rangle^c = \langle \psi_C | \Omega^\dagger X | \psi_B \rangle^c. \quad (7)$$

### C. The cumulant of the number 1

To complete the definition of the algebra of cumulant series we need to define the cumulant of the number 1. By formally putting the number of lambdas in the Definition 1 to zero we have

$$\langle x | 1 | y \rangle^c = \ln \langle x | y \rangle. \quad (8)$$

The usefulness of this definition comes from the point that the new object we just introduced satisfies the general expression for an infinitesimal transformation of a cumulant. It can be directly checked that

$$\langle \psi_A | 1 | \psi_B \rangle^c = \langle \psi_A | 1(1 + \delta S) | \psi_{B'} \rangle^c.$$

Therefore when doing transformations we need not to discriminate between the cumulant of the number 1 and "ordinary" cumulants.

### D. Superoperators

In parts of this article we use cumulants of superoperators, so we will repeat some considerations from [2]. A *superoperator* is an operator acting in the space of all operators, i.e. Liouville space. The cumulant of a superoperator  $D$  is defined in a way completely analogous to the ordinary cumulant. For instance:

$$\langle x | D | y \rangle^c = \frac{\partial}{\partial \lambda_{\lambda=0}} \ln \langle x | e^{\lambda D} \mathbf{1} | y \rangle. \quad (9)$$

Here  $\mathbf{1}$  is the unit operator of the Liouville space.

We see that the only difference is that we need to include the unit operator when defining cumulants.

For some operator  $H$  we introduce the superoperator  $L$ :  $L = [H, \dots]$ .

Cumulants containing  $L$  have the following property ([22])

**Statement 4** *For any cumulant expression  $G$  and for any operator  $A$  it is*

$$\langle GLA \rangle^c = \langle G(LA)^\bullet \rangle^c. \quad (10)$$

*Proof:*

The existence of  $G$  does not play any role in the following proof and so we omit  $G$  to simplify the writing.

$$\begin{aligned} \langle LA \rangle^c &= \frac{\partial^2}{\partial \lambda_1 \partial \lambda_2} \bigg|_{\lambda_1=\lambda_2=0} \ln \langle x | e^{\lambda_1 L} e^{\lambda_2 A} | y \rangle \\ &= \frac{\partial}{\partial \lambda_1} \frac{\partial}{\partial \lambda_2} \bigg|_{\lambda_1=\lambda_2=0} \ln \langle x | (1 + \lambda_1 L)(1 + \lambda_2 A) | y \rangle \\ &= \frac{\partial}{\partial \lambda_1} \frac{\partial}{\partial \lambda_2} \bigg|_{\lambda_1=\lambda_2=0} \ln \langle x | (1 + \lambda_1 \lambda_2 LA) | y \rangle = \frac{\partial}{\partial \lambda} \bigg|_{\lambda=0} \ln \langle x | (1 + \lambda LA) | y \rangle \end{aligned} \quad (11)$$

Here we wrote  $\lambda = \lambda_1 \lambda_2$ . For the second cumulant we have

$$\langle (LA)^\bullet \rangle^c = \frac{\partial}{\partial \lambda} \bigg|_{\lambda=0} \ln \langle x | e^{\lambda LA} | y \rangle = \frac{\partial}{\partial \lambda} \bigg|_{\lambda=0} \ln \langle x | (1 + \lambda LA) | y \rangle. \quad (12)$$

So the left and right sides of (10) are the same.

The superoperator  $L$  has the following property: if the right averaging vector in a cumulant is an eigenvector of  $H$  than  $L$  is equivalent to  $H$  in the cumulant expression. Indeed,  $L$  implies a commutation with  $H$ , and  $AH$  gives zero, because the right averaging vector is an eigenvector of  $H$ .

## E. Finite Temperatures

The above results can be extended to finite temperatures. Here the averaging implies taking a trace with some other operator (averaging operator). Therefore, we define the cumulant of a product of  $N$  operators as:

$$\langle A_1 \dots A_N \mid G \rangle^c = \frac{\partial}{\partial \lambda_1} \dots \frac{\partial}{\partial \lambda_N} \Big|_{\lambda_1 = \dots = \lambda_N = 0} \ln \text{Tr} \left( e^{\lambda_1 A_1} \dots e^{\lambda_N A_N} G \right). \quad (13)$$

Here  $G$  is an averaging operator. Considering infinitesimal transformations of  $G$  of the type  $G = e^{\delta S} G'$  we arrive at formulas which are identical to those of the zero temperature case.

Let us derive the cumulant expression for the free energy of the system.

Let be  $H = H_0 + H_1$  where  $H_0$  is an unperturbed Hamiltonian, and  $H_1$  is a perturbation.

Then

$$\begin{aligned} F &= -\beta \ln \text{Tr}(e^{-\beta H}) = -\beta \langle 1 \mid e^{-\beta H} \rangle^c \\ &= -\beta \langle 1 \mid e^{-\beta(L+H_1)} e^{-\beta H_0} \rangle^c = -\beta \langle e^{-\beta(L+H_1)} \mid e^{-\beta H_0} \rangle^c. \end{aligned} \quad (14)$$

In the first step we have used the definition of a cumulant of the number 1 and then transformed the averaging operator from  $e^{-\beta(L+H_1)} e^{-\beta H_0}$  to  $e^{-\beta H_0}$ .

Then  $\delta F = F - F_0 = -\beta \langle e^{-\beta(L+H_1)} - 1 \mid e^{-\beta H_0} \rangle^c$ .

This expression is analogous to the closed loop expansion of the free energy (thermodynamic potential) in field theory.

### III. APPLICATIONS OF CUMULANT GEOMETRY

Here we use the results obtained in the previous section to describe properties of a quantum system. Most of these results were obtained previously by using algebraic considerations [2–6]. Here we rederive them from a geometrical point of view.

#### A. Energy eigenvalues, orthogonality relations and expectation values

**Statement 5** *Let  $H$  be a Hamiltonian operator. Furthermore, let  $\psi$  be an eigenvector of this operator with an eigenvalue  $E$ . Let  $\psi_0$  be an arbitrary vector of Hilbert space  $\langle \psi_0 \mid \psi \rangle \neq 0$ , and  $\Omega$  a cumulant wave operator transforming  $\psi$  to  $\psi_0$ . Then for any formal series  $A$ , not including  $c$ -numbers, the following equations hold*

$$\langle \Psi_0 \mid H \Omega \mid \Psi_0 \rangle^c = E \quad (15)$$

$$\langle \Psi_0 | AH\Omega | \Psi_0 \rangle^c = 0. \quad (16)$$

*Proof:*

By taking equations (3), (4) and transforming the right averaging vector from  $\Psi$  to  $\Psi_0$  we immediately obtain (15), (16).

Using Statement 2 and transforming  $\Psi$  into  $\Psi_0$  we find that the opposite statement is also true, i.e., if  $\Omega$  transforms  $\Psi$  into  $\Psi_0$  and (16) holds for any  $A$  then  $\Psi$  is an eigenvector of  $H$ .

Next we consider expectation values of different physical quantities.

**Statement 6** *Let  $\Psi$  be a vector, with  $\langle \Psi | \Psi \rangle = 1$ , let  $\Psi_0$  be another vector and let  $\Omega$  be a wave operator transforming  $\Psi$  into  $\Psi_0$ . Then*

$$\langle \Psi | G | \Psi \rangle = \langle \Psi_0 | \Omega^\dagger G \Omega | \Psi_0 \rangle^c. \quad (17)$$

*Proof:*

First we note that  $\langle \Psi | G | \Psi \rangle = \langle \Psi | G | \Psi \rangle^c$ . Transforming the right and left averaging vectors from  $\Psi$  to  $\Psi_0$  we arrive at (17).

## B. Explicit forms of the $\Omega$ operator

We consider cases when the integration (6) can be done analytically.

**Statement 7** *Let  $\Psi_B = e^S \Psi_C$  where  $S$  is an operator of Liouville space.*

*Then one of the possible forms for the wave operator transforming  $\Psi_B$  into  $\Psi_C$  is*

$$\Omega = e^S. \quad (18)$$

*In the last expression  $e^S$  should be understood in terms of a series expansion.*

*Proof:*

We take  $\delta S_i$  in (6) as:

$$\delta S_i = S/N.$$

Then we have for  $\Omega$

$$\Omega = \lim_{N \rightarrow \infty} \prod_{i=1}^N (1 + S/N) = e^S.$$

We have used a representation of the formal exponential series known from algebra. It is possible to prove a more general statement:

**Statement 8** *Let  $\Psi_B = e^{g(S)}\Psi_C$  where  $S$  is an operator of Liouville space, and  $g(S)$  is an analytic function with  $g(0)=0$ .*

*Then one of the possible forms for a wave operator transforming  $\Psi_B$  to  $\Psi_C$  is*

$$\Omega = e^{g(S)}. \quad (19)$$

*In the last expression  $e^{g(S)}$  should be understood in terms of a series expansion.*

*Proof:*

We use for  $\delta S_i$  in (6) the expansion:

$$\delta S_i = g'(iS/N)S/N$$

Then we can write

$$\Omega = \lim_{N \rightarrow \infty} \prod_{i=1}^N \left[ 1 + \frac{S}{N} g' \left( \frac{iS}{N} \right) \right].$$

It is known from the theory of series expansions (see for instance [23]) that this expression tends to

$$\Omega = \exp [g(S)] \quad .$$

The question arises under which conditions an analytic function  $f(S)$  can be represented by  $e^{g(S)}$ . The theorem for Weierstrass products [23] states that a necessary and sufficient condition is that function  $f(s)$  does not have zeroes in the complex plane.

For instance, the function  $1 + S$  has a zero in the complex plane and therefore cannot be represented by  $e^{g(S)}$ . Therefore, we cannot state that if  $\Psi_B = 1 + S\Psi_C$  then  $\Omega = 1 + S$ .

Let us now rederive an operator  $\Omega$  transforming the unperturbed ground-state  $|\psi_0\rangle$  of the Hamiltonian  $H_0 + V$  to the true ground-state  $|\psi\rangle$  derived in [2]. We assume the nondegenerate case.

First we make a remark that

$$\lim_{t \rightarrow \infty} e^{-Ht} |\psi_0\rangle = e^{-Et} \langle \psi | \psi_0 \rangle |\psi\rangle. \quad (20)$$

Here  $E$  is the ground-state energy of  $H$ . We assume that  $|\psi\rangle$  and  $|\psi_0\rangle$  have nonzero overlap. Because cumulants do not depend on the norm of the averaging vectors the prefactor in front of  $|\psi\rangle$  is not important and we can write

$$\lim_{t \rightarrow \infty} e^{-Ht} |\psi_0\rangle = |\psi\rangle. \quad (21)$$

Then using (18) we write

$$\Omega = \lim_{t \rightarrow \infty} | e^{-Ht} \rangle. \quad (22)$$

Taking the Laplace transform with respect to the variable  $z$  and multiplying by  $z$  to get the constant part of the expression we obtain

$$\Omega = \lim_{z \rightarrow 0} | \frac{z}{z - H} \rangle = \lim_{z \rightarrow 0} | 1 + \frac{1}{z - H} H \rangle = \lim_{z \rightarrow 0} | 1 + \frac{1}{z - H} V \rangle. \quad (23)$$

This expression coincides with the one [2]. In the last line we took into account the fact that  $|\psi_0\rangle$  is an eigenvector of  $H_0$ .

### C. Wavefunction

Here we consider the question how to obtain the wavefunction from the  $\Omega$  operator.

**Statement 9** *Let  $\Psi$  and  $\Psi_0$  be vectors of Hilbert space, and  $\Omega$  be a cumulant wave operator transforming  $\Psi$  to  $\Psi_0$ . Then there exists an expression for  $\Psi$  through  $\Psi_0$  and  $\Omega$  that is be derived below.*

*Proof:*

We use the fact that

$$\nabla_{\Psi_0} \langle \Psi_0 | 1 | \Psi \rangle^c = \nabla_{\Psi_0} \ln \langle \Psi_0 | \Psi \rangle = \frac{| \Psi \rangle}{\langle \Psi_0 | \Psi \rangle} = | \Psi_{norm} \rangle.$$

Here 1 is number 1 and  $| \Psi_{norm} \rangle$  means that  $| \Psi \rangle$  is normalized by the condition  $\langle \Psi_0 | \Psi \rangle = 1$ .

By transforming the left side from  $\Psi$  to  $\Psi_0$  we have:

$$\Psi_{norm} = \nabla_{left \Psi_0} \langle \Psi_0 | \Omega | \Psi_0 \rangle^c. \quad (24)$$

Here  $left \Psi_0$  means that we should take the gradient only with respect to the left  $\Psi_0$ .

### D. Green Functions

In order to treat Green functions we need to generalize the definition of cumulants by including cases with the averaging operators inside.

We explain this extended definition by giving an example:

$$\langle u \underline{A} w \underline{B} \rangle_c = \frac{\partial}{\partial \lambda_1} \frac{\partial}{\partial \lambda_2} \ln \langle x | u e^{\lambda_1 A} w e^{\lambda_2 B} | y \rangle. \quad (25)$$

This is the cumulant of operators  $A$  and  $B$  with averaging vectors  $| x \rangle$  and  $| y \rangle$  outside and averaging operators  $u$  and  $w$  inside.

The usefulness of this definition is seen by noticing, that we can write a Matsubara Green's function [24] the following way (we assume  $\langle \psi | \psi \rangle = 1$ ):

$$\begin{aligned} R_{ij}(\tau) &= \langle \psi | c_i e^{\tau H} c_j^\dagger e^{-\tau H} | \psi \rangle = \langle \psi | c_i e^{\tau H} c_j^\dagger e^{-\tau H} | \psi \rangle - \langle \psi | c_i | \psi \rangle \langle \psi | c_j^\dagger | \psi \rangle = \\ &= \langle \psi | c_i e^{\tau H} c_j^\dagger e^{-\tau H} | \psi \rangle^c = \langle \psi | c_i e^{\tau L} c_j^\dagger | \psi \rangle^c. \end{aligned} \quad (26)$$

Therefore, we can write a Matsubara Green function as a 2-operator cumulant. We can find formulas for transformations of averaging operators which are similar to the formulas for transformations of averaging vectors.

As a result we obtain the following expression for the Laplace transform of  $R_{ij}$

$$R_{ij}(z) = (\Omega | (\frac{1}{z-L} c_i)^\bullet c_j^\dagger | \Omega). \quad (27)$$

This result coincides with the one obtained in [6,2] by resummation of a power series.

In a similar way expressions for higher-order Green functions can be obtained.

## E. Short-time propagators

The Diffusion Quantum Monte Carlo technique uses Feynman's path integration for the evaluation of physical properties of a system. An important issue is the quality of a *short-time propagator* by means of which we obtain the evolution of the system after a small period of time. M. Suzuki [25] first proposed to calculate improved short-time propagators using cumulant expansions. Below we explicitly calculate improved coordinate-momentum and coordinate-coordinate propagators for a general physical system with a Hamilton operator  $H = p^2/2 + V(q)$ . The *real-space propagator* is defined as a matrix element of the evolution operator between two  $\delta$ -functions representing the eigenstates of the position operator [26]. Because two delta functions situated at different points of the real space have zero overlap, we are not able to apply cumulants directly to the real space. The idea is then to extend the method used by Faddeev [27] to obtain the first-order propagator. First we calculate the phase-space propagator, and then by taking the Fourier transform come back to the real space.

The *phase-space propagator* is defined as [27]

$$F(p, q, t) = \langle p | e^{-iHt/\hbar} | q \rangle = \exp \left[ \langle p | e^{-iHt/\hbar} | q \rangle^c \right]. \quad (28)$$

Consider  $H = p^2/2 + V(q)$ . The above expression allows us to evaluate an improved short-time propagator up to any power of  $t$ . Let us calculate it to order  $t^2$ . Direct calculation gives:

$$F(p, q, t) = (2\pi)^{-1/2} \exp \left[ -ipq\hbar^{-1} - i(p^2/2 + V(q))t\hbar^{-1} - \frac{1}{4}(2p\hbar V'(q) - V''(q))t^2 \right]. \quad (29)$$

Going over to the  $(q', q'')$  propagator we have:

$$F(q', q'', t) = \langle q'' | e^{iHt} | q' \rangle = (2\pi)^{-1/2} \int e^{ipq''} F(p, q') dp. \quad (30)$$

By inserting (29) and evaluating the integral over  $p$  we obtain the short-time real space propagator:



$$F(q', q'', t) = \frac{1}{\sqrt{(2\pi i \hbar T)}} \exp \left[ i \frac{[q'' - q' + (1/2)t^2 V'(q')]^2}{2t\hbar} - itV(q')\hbar^{-1} - 1/4t^2 V''(q') \right]. \quad (31)$$

In a similar manner the next order short-time propagators can be computed.

Let us discuss the physical meaning of the expression (31). We have two additional terms in the propagator as compared to the usual leading order expression derived in [28]. The term  $(1/2)t^2 V'(q')$  corresponds to the fact that the velocity of the particle following a Feynman path is not constant, changing due to the force  $V'(q')$  and therefore leading to a correction of the kinetic energy term. The meaning of the term  $1/4t^2 V''(q')$  will be considered later.

Let us use the above results to obtain a high-temperature expansion for the partition function of a quantum system.

The partition function is defined as [28]:

$$Z = \text{Tr} \exp(-\beta H) = \int \langle q | \exp(-\beta H) | q \rangle dq. \quad (32)$$

For small  $\beta$  we can use the expansion (31) setting  $t = -i\beta$ . Then we have to order  $\beta^2$ :

$$Z = \frac{1}{\sqrt{(2\pi \hbar^2 \beta)}} \int \exp \left[ -\beta V(q) - (1/4)\hbar^2 \beta^2 V''(q) \right] dq. \quad (33)$$

To the first order in  $\beta$  we obtain a classical expression for a partition function, this means that for high temperatures the average energy of the system is large and we can neglect quantisation effects.

Let us discuss the meaning of the correction  $1/4\hbar^2 \beta^2 V''(q)$ . Suppose the potential  $V(q)$  has a very high but very narrow peak. Then the region of the peak will be prohibited in a classical theory because  $V(q)$  is large. On the other hand, for the quantum case there will be some probability for the system to be in the region of the peak due to tunnelling. For a high and narrow peak  $V''(q)$  will be large and negative. Now looking at the expression (33) we see that  $1/4\hbar^2 \beta^2 V''(q)$  has then a sign opposite to  $\beta V(q)$  so the potential is effectively smeared out. Therefore, we see that  $1/4\hbar^2 \beta^2 V''(q)$  term describes an effective smearing of the potential due to the quantum tunnelling.

The expansion for a partition function obtained above is a high temperature expansion (in powers of  $\beta$ ). We note that this expansion does not coincide with the quasiclassical expansion (in powers of  $\hbar$ ). Although both types of expansions give the classical formula as the leading term, the higher-order terms are different. The expansion in powers of  $\hbar$  was first obtained by Wigner [29]. To the second order in  $\hbar$  it can be written as:

$$Z = \frac{1}{\sqrt{(2\pi\hbar^2\beta)}} \int \exp \left[ -\beta V(q) - (1/12)\hbar^2\beta^2 V''(q) + (1/24)\hbar^2\beta^3 V'(q)^2 \right] dq. \quad (34)$$

The formulas for improved short-time propagators can be useful to improve the speed and the precision of numerical Quantum Monte Carlo calculations [25]. They could also improve analytical calculations that make use of short-time propagators.

We remark that the above technique applies only when the short-time propagator has a well-defined Fourier transform with respect to the coordinate. This is usually satisfied for potentials approaching zero or a constant at infinite distance. This condition includes the majority of potentials used for Monte Carlo calculations of quantum gases and liquids. The case when the propagator cannot be Fourier transformed with respect to the coordinate is subject to future considerations.

## IV. METHOD OF INCREMENTS

### A. Derivation of the Method of Increments starting from Faddeev's Equations

It happens frequently that we deal with a Hamiltonian consisting of different parts and that these parts considered separately can be solved analytically or numerically.

The first example of such a situation is the *3-body problem*. Three particles interact with each other by two-particle potentials. Considering each pair of particles separately we face a 2-body problem which can be solved analytically. Then the question is how we can use the information given by these solutions to construct an approximation to the solution of the whole 3-body problem.

The second example are quantum chemistry calculations where we need to find an approximate solution for a large molecule or a cluster having available numerical calculations for its subparts, i.e., chemical bonds.

For the 3-body problem L. D. Faddeev invented *coupled integral equations* that connect the unknown 3-body scattering matrix to 2-body scattering matrices that can be found analytically [15], [16].

In quantum chemistry the *method of increments* is well known, that expresses the ground-state energy in terms of a sum of local increments given by sets of 1, 2, 3 etc. chemical bonds.

Below we show that Faddeev's equations and the method of increments are closely related. The increment method can be obtained as a leading order approximation to *cumulant Faddeev-like equations* that we derive below.

We start by writing the wave operator in the form [2],

$$|\Omega\rangle = \lim_{z \rightarrow 0} \left| 1 + \frac{1}{z - H} V \right\rangle. \quad (35)$$

We also define a scattering operator  $S$ , which is small for small  $V$ ,

$$S = \Omega - 1 = \lim_{z \rightarrow 0} \sum_{n=1}^{\infty} \left| \left( \frac{1}{z - H_0} V \right)^n \right\rangle. \quad (36)$$

Let us first consider the case when the perturbation consists of three parts.

**Statement 10** *Consider a Hamiltonian with three perturbations,  $H_1$ ,  $H_2$  and  $H_3$*

$$H = H_0 + H_1 + H_2 + H_3. \quad (37)$$

*Let  $S_1$ ,  $S_2$ ,  $S_3$  be scattering operators for  $H_0 + H_1$ ,  $H_0 + H_2$  and  $H_0 + H_3$  respectively.*

*Then the scattering operator  $S$  of the Hamiltonian  $H$  can be found from the solution of the formal equations*

$$\begin{aligned} T_1 &= S_1 (1 + T_2 + T_3) \\ T_2 &= S_2 (1 + T_1 + T_3) \\ T_3 &= S_3 (1 + T_1 + T_2) \\ S &= T_1 + T_2 + T_3. \end{aligned} \quad (38)$$

*Proof:*

We write  $S$  in a power series as

$$S = \sum_{n=1}^{\infty} \left( \frac{1}{z - H_0} (H_1 + H_2 + H_3) \right)^n \quad (39)$$

and define

$$A_1 = \frac{1}{z - H_0} H_1, \quad A_2 = \frac{1}{z - H_0} H_2, \quad A_3 = \frac{1}{z - H_0} H_3. \quad (40)$$

Then

$$S = \sum_{n=1}^{\infty} (A_1 + A_2 + A_3)^n = \sum A_1 \dots + \sum A_2 \dots + \sum A_3 \dots = T_1 + T_2 + T_3. \quad (41)$$

We divided the terms in the power series into three groups, the terms in the first group begin with  $A_1$ , the ones in the second group with  $A_2$ , in the third group with  $A_3$ . We call these three sums  $T_1$ ,  $T_2$ ,  $T_3$ .

We rewrite  $T_1$  in the form

$$\begin{aligned} T_1 &= (A_1 + A_1^2 + \dots) + (A_1 + A_1^2 + \dots) A_2 + (A_1 + A_1^2 + \dots) A_3 + \dots = \\ &= (A_1 + A_1^2 + \dots) (1 + T_2 + T_3). \end{aligned} \quad (42)$$

The first bracket defines  $S_1$ . The expressions for  $T_2$ ,  $T_3$  are similar. This results in Faddeev's equations (38).

In the original work of Faddeev  $S_1$ ,  $S_2$ ,  $S_3$  correspond to two-body scattering matrices coming from three pairs of particles in the 3-body problem, and  $S$  corresponds to the unknown 3-body scattering matrix.

We easily generalize our equations to the case when the perturbation has  $N$  parts, in that case we have  $N$  equations of the type

$$T_i = S_i \left( 1 + \sum_{j \neq i} T_j \right). \quad (43)$$

Assuming  $S_i$  to be small, the equations can be solved by iterations. Then  $S$  is given by (41).

In the leading approximation we have

$$T_i = S_i, \quad S = \sum S_i. \quad (44)$$

By using the formulas  $E = (H | \Omega)$  and  $\Omega = 1 + S$  where  $E$  is the ground-state energy of  $H$  we can write

$$\delta E = E - E_0 = \sum \delta E_i, \quad (45)$$

$$\delta E_i = (H | S_i). \quad (46)$$

Here  $E_0$  is the ground-state energy of  $H_0$ . The equation (45) gives the simplest example of a increment method. We call the  $\delta E_i$ 's first-order increments.

Let us state the result: we start from Faddeev's equations, solve them in the leading order approximation and obtain a first-order increment method.

Below we show that we can formulate higher-order Faddeev's equations. Taking the  $N$ -th order Faddeev's equation and solving it in the leading order approximation we obtain exactly the  $N$ -th order increment method. Therefore Faddeev's equations and increment methods are closely related.

As an example we derive the second-order Faddeev's equations. We again take a Hamiltonian consisting of  $H_0$  part and  $N$  perturbations

$$H = H_0 + H_1 + \dots + H_N. \quad (47)$$

But now we additionally assume that we can solve analytically or numerically all the Hamiltonians of the form  $H_0 + H_i + H_j$ , i.e., that we know the scattering operators  $S_{ij}$  for these Hamiltonians.

Then we write again the expression for  $S$ ,

$$\begin{aligned} S &= \sum_{n=1}^{\infty} (A_1 + \dots + A_N)^n = \\ &= \sum A_1 \dots A_2 \dots + \sum A_2 \dots A_3 \dots + \sum A_1 \dots A_3 \dots + \dots + \sum_{n=1}^{\infty} A_1^n + \dots \sum_{n=1}^{\infty} A_N^n = \\ &= \sum_{1 \leq i, j \leq N} T_{ij} + \sum_{n=1}^{\infty} S_i. \end{aligned} \quad (48)$$

This resummation is more sophisticated and needs explanations. First, we open brackets in the sum in order to obtain a power series with respect to  $A_i$ 's. For each term in this power

series we look for the first two letters in it, and regroup terms according to this property. For example,  $T_{1,2}$  will be the sum of all terms in the power series having  $A_1$  and  $A_2$  as the first two letters, so that ,e.g., the term  $A_1^3 A_2^2 A_4$  is included in  $T_{1,2}$ .

We are still left with terms containing only one letter like  $A_2^4$ . These terms are not contained in any of  $T_{ij}$ 's so we sum them separately, this explains the result of (48).

Now we consider  $T_{1,2}$ :

$$\begin{aligned} T_{1,2} &= (A_1 A_2 + A_1 A_2^2 + A_1^2 A_2 + A_1 A_2 A_1 + \dots) \left( 1 + \sum_{(i,j) \neq (1,2)} T_{ij} + \sum_{i \neq 1,2} S_i \right) = \\ &= (S_{1,2} - S_1 - S_2) \left( 1 + \sum_{(i,j) \neq (1,2)} T_{ij} + \sum_{i \neq 1,2} S_i \right). \end{aligned} \quad (49)$$

This result is obtained by considerations similar to the previous ones. The first bracket is a sum of all possible terms consisting of  $A_1$ 's and  $A_2$ 's only. The second bracket is a sum of all possible terms that do not have  $A_1$  and  $A_2$  as the first two letters.  $S_{1,2}$  denotes the scattering operator for the Hamiltonian  $H_0 + H_1 + H_2$ .

The similar equations are obtained for all other  $T_{ij}$ . Together with (48) these equations give the second-order cumulant Faddeev's equations.

Taking again the leading approximation for the equations we have:

$$S = \sum_i S_i + \sum_{i,j} K_{ij} \quad (50)$$

where

$$K_{ij} = S_{ij} - S_i - S_j. \quad (51)$$

Here  $K_{ij}$  is a cumulant operator corresponding to the second-order increment.

Using the formula for the ground state energy  $E = (H | \Omega)$  we arrive at an expression up to the second-order increment expression

$$\delta E = \sum_i \delta E_i + \sum_{i,j} \delta E_{ij}. \quad (52)$$

The second order increments  $\delta E_{ij}$  are given by

$$\delta E_{ij} = (H | K_{ij}) = (H | S_{ij}) - \delta E_i - \delta E_j \quad (53)$$

By continuing this procedure and taking the leading approximation to the next contribution we end up with the third-order cumulant expression for  $S$

$$S = \sum_i S_i + \sum_{i,j} K_{i,j} + \sum_{i,j,k} L_{ijk} \quad (54)$$

$$L_{ijk} = S_{ijk} - K_{ij} - K_{ik} - K_{jk} - K_i - K_j - K_k. \quad (55)$$

Again this expression agrees up to third-order with the energy expression of the increment method. The same holds true for higher-order contributions.

Next we consider the error when terms up to the  $N$ -th order increment are taken into account. From (49) we see that the first bracket is of second order in the perturbation, while the remaining term that we omit in the leading-order approximation is of first order, therefore making a leading-order approximation to the equations finally leads to an error  $S$  and  $E$  which is of third order. Generally, inclusion of  $N$ th order increments will lead to an error which is of the order  $N + 1$ .

Actually, the increment expansion may converge much more rapidly and the perturbation does not need to be small.

Consider for instance a large molecule. The term omitted by the leading order approximation to Faddeev's equations can make a significant change to the result only when all its parts add coherently; otherwise its contribution will be close to zero. Consider a term corresponding to a set of  $K$  chemical bonds. If the spatial extent of this set is larger than a characteristic length we called the correlation length  $\lambda$ , then the omitted terms in the Faddeev's equation will sum incoherently and can be neglected. Therefore we can terminate an expansion of the correlation energy in terms of increments when the spatial extent of a set of bonds is of the order of the correlation length. This is in accordance with the well known idea, that the minimum size to which we can reduce a system not changing its macroscopic properties is dictated by the correlation length [30]. In order to formulate it more rigorously we may state that the macroscopic properties of an infinite solid can be described by an incremental expansion with increments taken up to the correlation length. Therefore

incremental methods will work efficiently for systems having a moderate correlation length, like semiconductors [11].

### B. Method of increments for excited states

In the following we formulate a method of increments for excited states. We begin with a nondegenerate unperturbed Hamiltonian, so perturbations do not split excitation energies, instead they only shift them.

Consider again as an example a Hamiltonian with three perturbations  $H = H_0 + H_1 + H_2 + H_3$ .

Consider an excited state  $E_i$  of  $H_0$ . We want to show that the incremental method for an excited state can be formulated in a similar way as done before for the ground-state .

We start from a formula derived in [4] for the excited states of a Hamiltonian:

$$E_i = \langle \psi_i | H \Omega | \psi_i \rangle^c. \quad (56)$$

Here  $|\psi_i\rangle$  is an excited state of  $H_0$  having an overlap of more than 1/2 with the true excited state we are looking for (for details see [4]).

Let us apply the incremental expression for  $\Omega$  to this formula.

To first order of the incremental expansion (see (44)) we obtain

$$\delta E_i = \delta E_{i,1} + \delta E_{i,2} + \delta E_{i,3}. \quad (57)$$

Here  $\delta E_{i,1}, \delta E_{i,2}, \delta E_{i,3}$  are increments corresponding to the excited state  $i$ ,

$$\delta E_{i,j} = \langle \psi_i | H S_i | \psi_i \rangle^c. \quad (58)$$

In the second order of the incremental expansion we find:

$$\delta E_i = \delta E_{i,1} + \delta E_{i,2} + \delta E_{i,3} + \delta E_{i,1,2} + \delta E_{i,2,3} + \delta E_{i,1,3} \quad (59)$$

where  $\delta E_{i,1,2} = \langle \psi_i | H S_{1,2} | \psi_i \rangle^c - \delta E_{i,1} - \delta E_{i,2}$  etc.

In an analogous way next order increment expressions can be obtained.



Let us consider as an example of an increment calculation the valence band calculations done in [31].

In a first step self-consistent field CSCF calculations are done and the energy bands in SCF approximation are obtained. Then the SCF states are transformed into Wannier states (localized orbitals) and the residual part of the interaction  $H_{res} = H - H_{SCF}$  is expressed in terms of matrix elements between the localized bonds.

The increment method up to forth order was used to obtain the valence band. In this case SCF hamiltonian plays the role of  $H_0$  and the matrix elements of the residual Hamiltonian between pairs of localized bonds play role of perturbations. In the calculations increments corresponding to NN (nearest neighbours) and NNN (next-nearest neighbours) were retained and the effect of more distant correlations was approximated by introducing a polarizable continuum.

The results have been shown to describe with a good accuracy the reduction of the valence bonds of diamond due to correlations [31].

## V. CONCLUSIONS

In this article we considered the question, how geometrical methods can be used to formulate the theory of cumulant expansions. Cumulant geometry simplifies the proofs of many expressions obtained before by cumulant algebra and makes them transparent.

Then we studied applications of the cumulant technique to short-time propagators and to the method of increments. In both cases the use of cumulants is a natural choice. A hierarchy of cumulant Faddeev-like equations was generated and a method of increments for excited states was established.

Future directions of research will include diverse applications of the cumulant technique to solid state theory. A particularly interesting question there is how properties of the infinite solid can be related to properties of a finite cluster. This question is of outmost importance for all numerical calculations.

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